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The Meisner Minute

Editorial by Bob Meisner

This past quarter brought with it significant change and progress.

In May, Michael Strayer and I formed the Exascale Initiative Steering Committee (EISC) that recognizes the need for ASC and the Office of Advanced Scientific Computing Research in the Office of Science to collaborate if we are to be successful at achieving exascale computing by the end of next decade. The committee is comprised of representatives from Lawrence Livermore, Los Alamos, Sandia, Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge and Pacific Northwest national laboratories.

We have tasked the EISC with developing a science case for exascale computing and a high level roadmap. This information will assist us in planning the research and development activities necessary to field an exascale system and host initial DOE application codes by 2018. Of course, this is a difficult challenge. The timeframe is short, and there are many obstacles to be overcome, including power requirements, scalability, fault tolerance, memory limitations, and cost. Initial planning and presentations to DOE senior management will take place over the next few months. This next step is an important one for the program and I am very pleased that we are able to do it in collaboration with the Office of Science.

We are also seeing some staffing changes at HQ. Njema Frazier has moved on to direct the International Program Management Division, under Dimitri Kusnezov. The breadth of work formerly handled by her is being distributed across existing ASC staff as well as Trieu Truong, who came to us from the Directed Stockpile Work (DSW), Engineering Campaign. Trieu’s responsibilities will lie primarily in verification and validation with a significant mandate to integrate with the science campaigns and DSW.

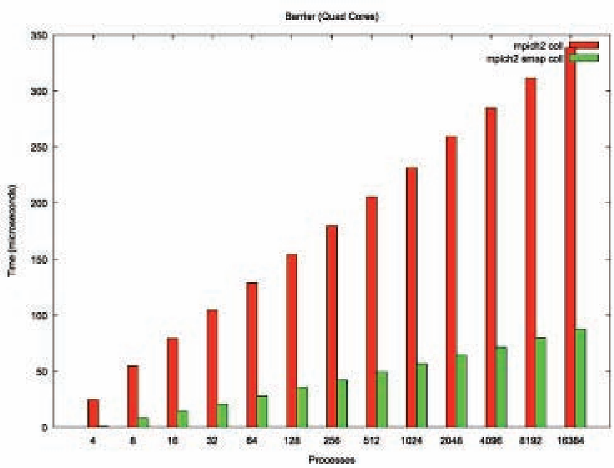
The new Deputy Director for ASC will be Doug Wade who joins us from the NA-10 Strategic Planning, Resources, and Integration Office. Doug comes to us with a nuclear engineering, strategic planning, and R&D management background and nearly 20 years of experience within Defense Programs. We also have two detailees from LLNL. Dan Nikkel is taking a year off from his duties as the Deputy Program Leader for Physics and Engineering Models (PEM), and Deputy of the Dynamic Materials Properties Science Campaign to focus on tri-lab execution of the PEM elements of the program. Des Pilkington, who became a US citizen this past year, comes to us with an extensive background in code development and will help direct activities that lead us to predictive capability. Finally, Beverly Berger has rejoined the program on a detail to work on educational outreach.

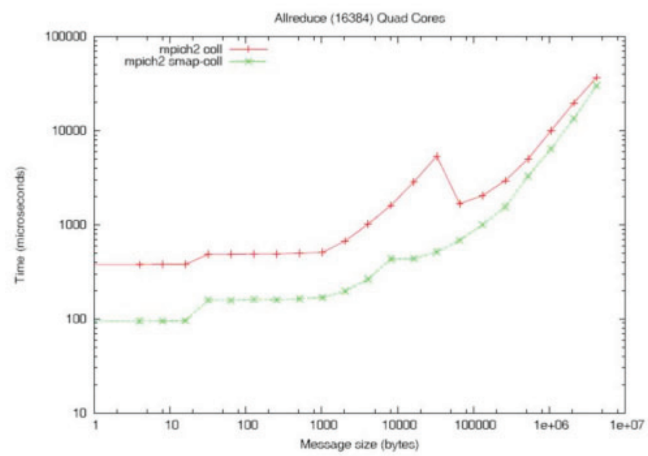
Although this quarter’s update reflects immense change, we maintain our laser focus on predicting with confidence, a vision critically dependent on exascale computing. Even with all the changes at headquarters, we understand our obligation to nuclear deterrence and continue to enthusiastically advocate for the program. But, the real fun and all of the laudable achievements happen at the labs. Your contribution to national security and the safety, reliability, and performance of the stockpile is critical to our national security and is exemplary. Even through this period of change, together we make an unbeatable team.

Sandia Wins a 2009 R&D 100 Award for Catamount Light Weight OS for Multi-Core Processors

The latest version of the Catamount Operating System (OS) has been dubbed “Catamount N-Way” because it supports “N” cores per compute node. It exploits existing features of multi-core processors to deliver significant improvements in data access performance for parallel computing applications. Catamount currently runs on the Red Storm Supercomputer located at Sandia, which has 6720 dual-core and 6240 quad-core nodes.

One of the significant enhancements in this operating system is a new technique, called SMARTMAP, that targets memory bandwidth, arguably the most important area of performance in scientific parallel computing. It cuts in half the required memory bandwidth for intra-node message passing. Red Storm's





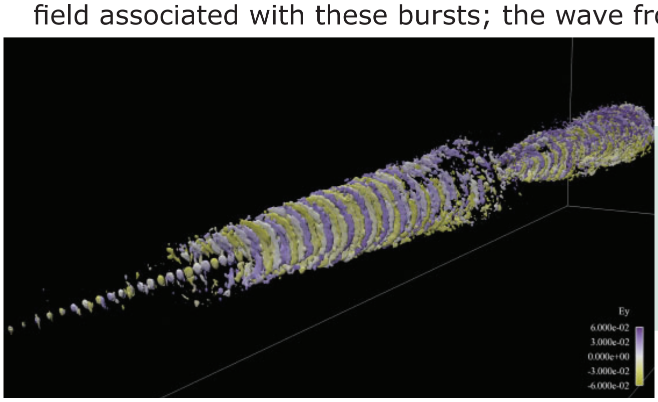
production MPI library, MPICH, has been modified to employ SMARTMAP to do in-place, collective operations for critical functions.

The graphs above show the reduced completion times for Allreduce and Barrier. This version of the operating system provides the ability for the majority of the scientific parallel applications to more effectively use multi-core processors, thereby extending the lifetime of current applications without any changes to the application itself.

Largest Ever Plasma Particle-in-Cell Calculation Enabled by Roadrunner

In support of the National Ignition Campaign (NIF) and Laboratory Directed Research and Development, the Roadrunner supercomputer (located at Los Alamos National Laboratory [LANL]) has been used during its open-science stabilization phase to perform fully kinetic plasma simulations of laser-plasma interaction (LPI) under conditions encountered in inertial confinement fusion experiments on NIF. f/8 laser speckles were modeled under NIF plasma conditions to understand onset and saturation of Raman backscatter (SRS) instability. See the schematic showing Lawrence Livermore National Laboratory pf3D modeling of laser and Hydra modeling of ignition caption with LANL VPIC simulation volume.

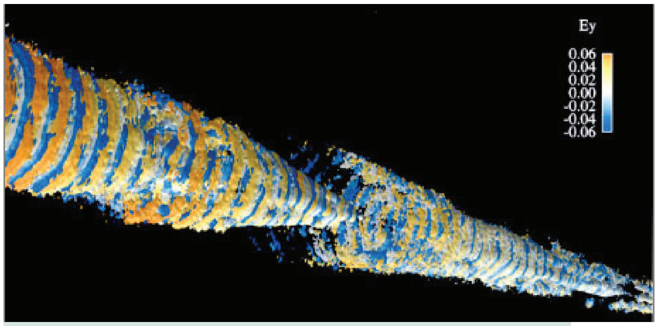
These simulations employ the VPIC particle-in-cell code and are among the most ambitious ever performed. The largest of these was run on the full Roadrunner system and employed a record 0.4 trillion particles, over 2 billion cells, and ran for nearly 58,160 time steps (nearly 1019 floating point operations), long enough for two bursts of SRS. The simulations showed that nonlinear self-focusing governs SRS saturation and limits the amount of laser backscatter. The figures show isosurfaces of electrostatic field associated with these bursts; the wave fronts exhibit bending or "bowing," arising from nonlinear particle trapping, as well as self-focusing, which breaks up the phase fronts.



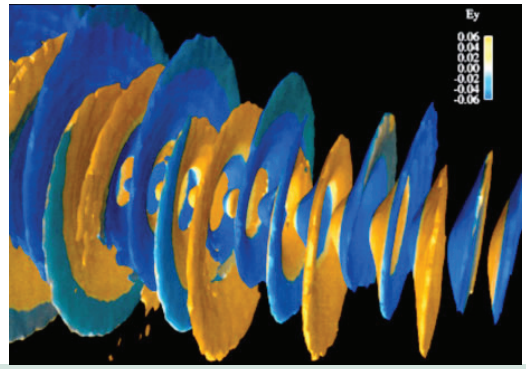
Isosurfaces of electrostatic field associated with stimulated Raman scattering. The wave fronts exhibit bending or "bowing," arising from non-linear particle trapping, as well as self-focusing, which breaks up the phase fronts.

From these basic science simulations, researchers are able to understand better the essential nature of LPI saturation. From this experience, we expect that Roadrunner will for the first time enable three-dimensional ab initio simulations of LPI with rapid turn-around and allow us to model LPI over a range of conditions encountered in fusion ignition experiments.

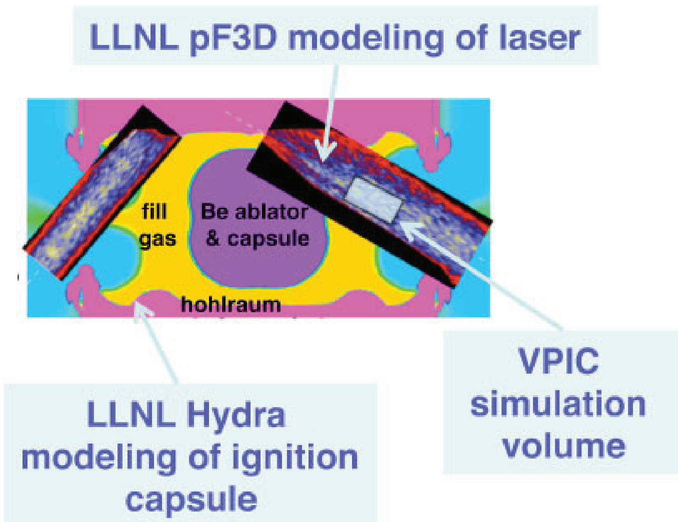
For more information about this Roadrunner open science project, go to "Saturation of Backward Stimulated Scattering of Laser in the Collisional Regime" at http://www.lanl.gov/orgs/hpc/roadrunner/pdfs/openscience/Abstracts3%201.pdf.



LANL VPIC ab initio modeling of laser plasma interaction. The largest ever plasma particle-in-cell calculation, enabled by Roadrunner.



LANL VPIC modeling of laser plasma interaction on full Roadrunner system.



Understanding Raman backscatter (SRS) is critical to the success of inertial fusion on the National Ignition Facility.

Validation of W80 Abnormal Mechanical Model to Probabilistically Assess Nuclear Safety

In a study funded by the Advanced Simulation and Computing (ASC) Program, a model of the W80 is undergoing verification and validation (V&V) for probabilistic assessment of nuclear safety in abnormal mechanical environments such as handling drop accidents.

Underpinning this project are the V&V practices and computational tools developed by the ASC program, including the use of the Predictive Capability Maturity Model (PCMM) to prioritize activities, Design Through Analysis Realization Team (DART) tools to manage the complex system model and SIERRA mechanics codes to perform simulations.

Important data on material behavior have been generated by Campaign 6-funded material testing. Peer review of the study began with a mid-FY evaluation by a panel of experts. This project is supporting the 2009 and 2010 W80 Annual Assessment Reports and, beginning in FY10, will provide initial quantified margins and uncertainties (QMU) for nuclear studies.

Early Science Runs on Dawn Push the Forefront of Predictive Simulation

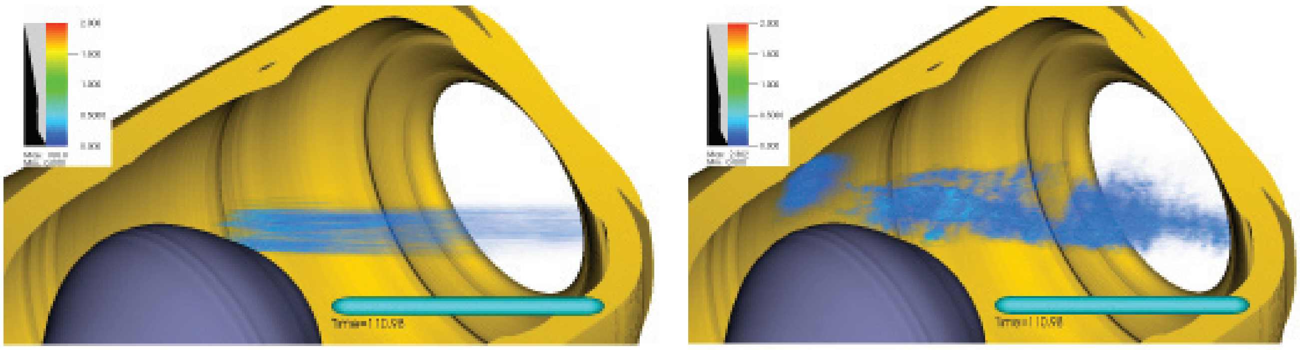
The 500-teraFLOPS ASC Sequoia Initial Delivery System (Dawn), an IBM machine of the same lineage as BlueGene/L, has immediately proved itself useful as several initial science results—performed from April through August—demonstrated ground-breaking science, enhanced code performance, and some of the highest resolution, largest simulations ever run in their respective scientific field.

Delivered to the Lawrence Livermore National Laboratory in January and February, Dawn (an IBM Blue Gene/P system) will lay the applications foundation for multi-petaFLOPS computing on Sequoia, a 20-petaFLOPS IBM system to be delivered in late 2011.

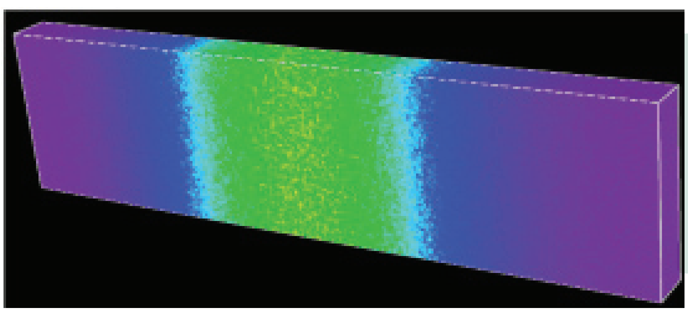
All three ASC labs—Lawrence Livermore, Los Alamos, and Sandia—have been busy using Dawn for the past five months and have been generating exciting new results across a broad spectrum of applications.

"The rapidly increasing performance of new supercomputers, such as Dawn, allows us to perform calculations unimaginable only a few years ago," said Denise Hinkel, AX Division's Plasma Theory Group Leader at LLNL. "Today's supercomputers are the enabling technology for predictive laser-plasma interaction modeling, and recent large-scale simulations on Dawn are helping guide focal-spot-sized decisions for the National Ignition Facility (NIF) beams and helping with ignition design optimization."

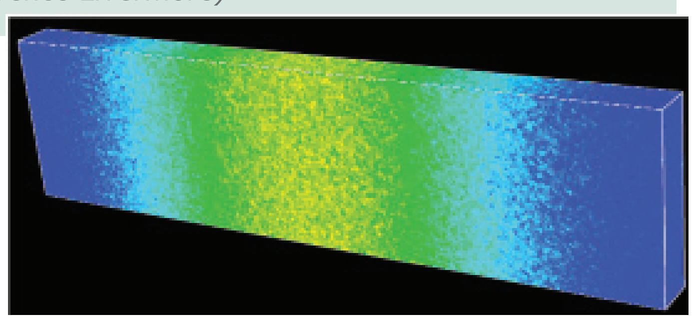
Below are examples of NIF laser and other simulations recently run on Dawn.

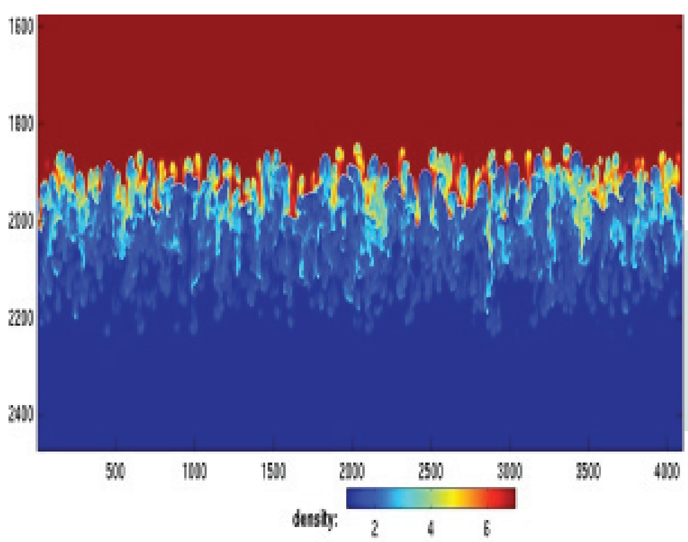


Laser beam propagation simulation showing simulated backscatter inside an ignition target (left panel: laser light resonantly scatters off ion acoustic waves; right panel: laser light resonantly scatters off electron plasma waves). Such simulations help to optimize NIF target performance. (Lawrence Livermore)

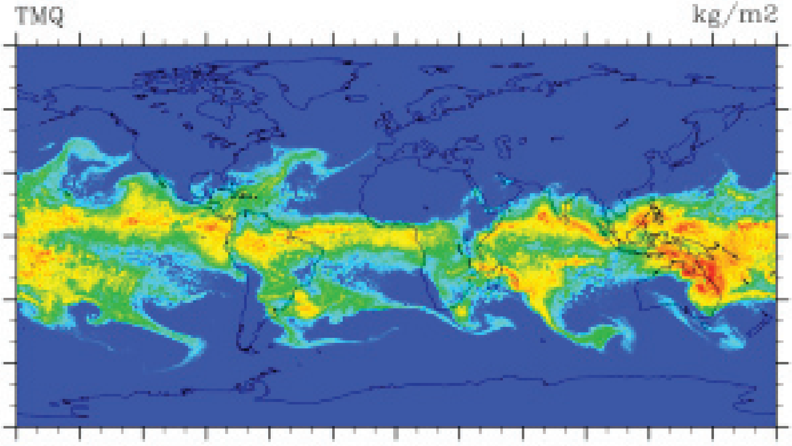


Evolution of electron temperature due to heating from a high-energy beam heating in a charged particle plasma-beam interaction simulation, providing insight about interactions that might occur in a fusion fast ignition experiment. (Lawrence Livermore)

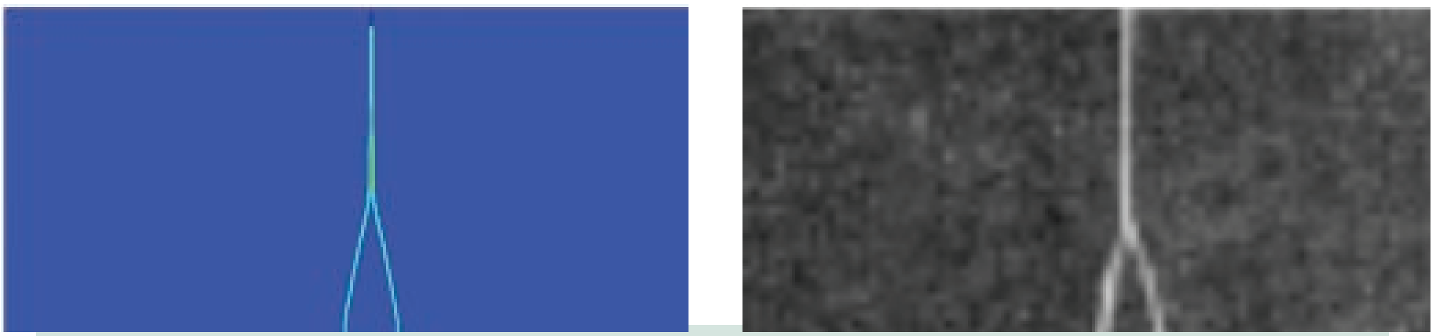




Vertical slice through Rayleigh-Taylor instability—important in many science applications—layer showing clear asymmetry with "spikes" falling on the light fluid side and "bubbles" rising on the heavy fluid side. (Los Alamos)



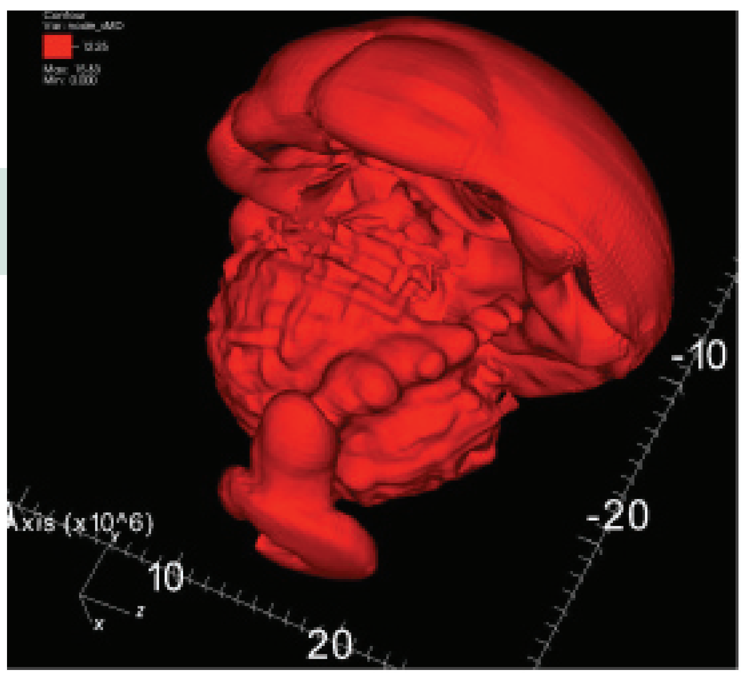
Snapshot of precipitable water in the Earth's atmosphere. High resolution climate models are key to obtaining information of sufficient resolution to assess national security and societal impacts of climate change. (Sandia)



Comparison of Dawn simulation (left) and physical experiment (right) of glass crack patterns. This simulation of dynamic brittle fracture is critical in the understanding of crack propagation using new peridynamics simulations. (Sandia)

VisIt Performance Reaches New Heights

Three weeks after HPCwire lauded Lawrence Livermore National Laboratory's (LLNL) VisIt visualization software for tackling datasets up to 2 trillion zones, VisIt ran on the Dawn supercomputer and eclipsed 4 trillion zones.



Isocontour of 4 trillion zones resampled from a supernova calculation.

A team of Department of Energy (DOE) researchers from LLNL, Lawrence Berkeley National Laboratory (LBNL), and Oak Ridge National Laboratory (ORNL) ran a series of experiments with VisIt using 8,000 to 32,000 processing cores to see if VisIt could tackle datasets ranging from 500 billion to 2 trillion zones, or grid points. The greater the number of grid points, the more detailed the visualizations that VisIt can produce. Running on some of the world's most powerful supercomputers, VisIt was able to process datasets far larger than those currently produced by scientists, ensuring that VisIt is well prepared for the future.

Porting VisIt to Dawn was a multistep process, including cross-compiling VisIt's third-party dependencies for Dawn's compute nodes, changing VisIt's build system to focus on the compute engine since it is the piece that runs on Dawn, and eliminating runtime crashes caused by misconfigured libraries and removing more unsupported dependencies in the code.

Once VisIt was running on Dawn, bottlenecks were eliminated and bugs fixed. This included enhancing VisIt's plugin system and changing how VisIt communicates work among available processors (fewer large chunks instead of many small chunks). How VisIt reads spatial extents for some of its file readers was also altered to increase the amount of memory available for other data. Additional work included optimizing VisIt for the IBM compiler to generate more efficient code, and rewriting the slow parts of the code to increase VisIt's overall performance.

The work is part of an effort known as the Visualization and Analytics Center for Enabling Technologies (VACET), which was established by DOE in 2006 and is an integral part of the VisIt development effort. VACET includes researchers from UC Davis and the University of Utah, as well as Lawrence Berkeley National Laboratory (LBNL), LLNL and Oak Ridge National Laboratory (ORNL), and is part of DOE's Scientific Discovery through Advanced Computing (SciDAC) program.Complete story…

New Uncertainty Quantification Method Models Random Fields in Weapon Applications

A new uncertainty quantification (UQ) capability has been developed to model random surface contact and friction in mechanical joints. This capability is needed to model accurately the behavior of weapon components and subsystems when subject to structural vibration environments such as those that occur in a warhead during atmospheric re-entry.

This "random field" modeling capability was demonstrated on a bolted flange structure that is representative of actual weapon hardware. Simulations of the structural response of the hardware were conducted with Sandia's SIERRA simulation software, along with the advanced UQ capabilities of Sandia's DAKOTA software.

In the future, this modeling capability will be generalized across more of the SIERRA modules, so that random fields can be modeled in many other Sandia weapon and non-weapon applications, e.g., spatial and temporal random external pressure loads on re-entry flight vehicles, and, heterogeneous subsurface geology modeling for carbon dioxide sequestration studies. The ASC program has funded the SIERRA and DAKOTA development, as well as the UQ study.

Los Alamos' Roadrunner Permitting VPIC Simulations of Unprecedented Scale

Magnetic reconnection is a basic plasma process involving the explosive conversion of magnetic field energy into particle kinetic energy, including high-speed flows, thermal heating, and highly energetic particles. This process is thought to play an important role in a wide variety of applications ranging from solar flares, to the Earth's magnetosphere, to magnetic fusion devices. Three-dimensional simulations of magnetic reconnection are computationally challenging due to the large separation of spatial and temporal scales inherent to most applications. This is particularly true for kinetic simulations where both ion and electron kinetic scales must be fully resolved.

During the Roadrunner open science campaign, researchers at LANL employed the fully kinetic plasma simulation code VPIC to address some outstanding questions regarding 3D evolution of reconnection layers in kinetic regimes. These simulation efforts focused on two basic types of configurations. First, the team employed open boundary conditions to model magnetic reconnection in large open systems for application to space and astrophysical plasmas, which are typically in highly collisionless regimes. Second, the team implemented experimental boundary conditions relevant to the Magnetic Reconnection experiment (MRX) in order to allow direct validation comparisons regarding the kinetic structure and dynamics of the reconnection layer. These simulations included a Monte Carlo treatment of the Fokker-Planck collision operator in order to rigorously model the influence of weak Coulomb collisions in the experiment.

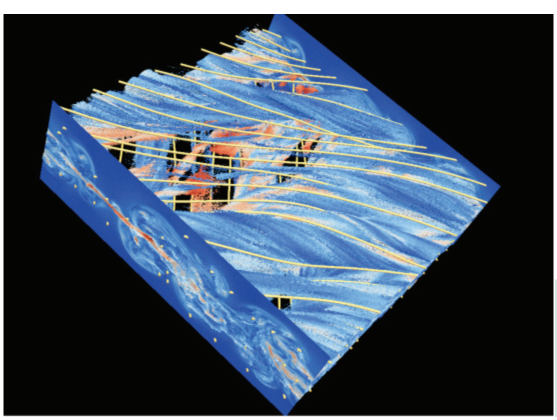
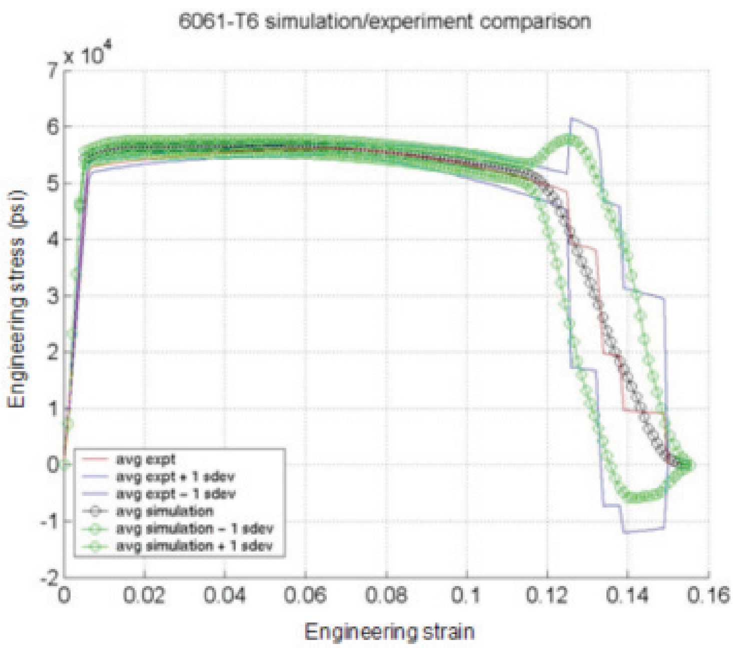


Image from VPIC open-science study showing interacting flux ropes forming across the reconnection layer. These results are consistent with recent theoretical predictions.

Los Alamos researchers were successful in completing a series of simulations for both types of problems using upwards of 4096 ranks (1/3 of full machine). These simulations are nearly a factor of ~100x larger than most researchers are presently able to study, and are already leading to a range of new scientific insights regarding the complex interplay of plasma instabilities with the 3D evolution of reconnection layers. Key new results concern the evolution of current-driven instabilities on the structure and evolution, along with the formation and interaction of flux ropes in large systems, as seen in the figure. These new results will be described in series of publications and invited talks, starting this fall.

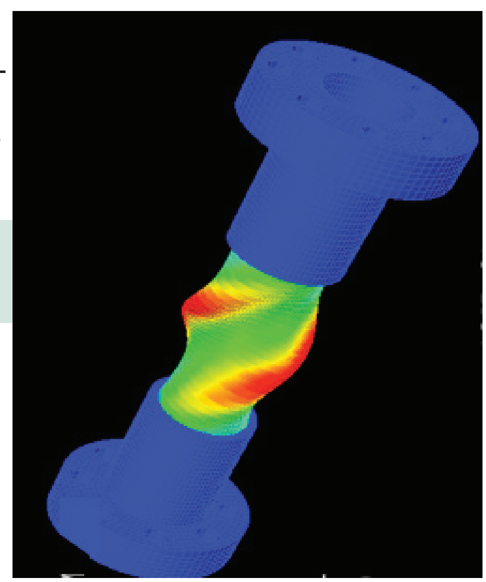
Material Response Variability Characterized and Propagated in Non-linear Structural Response Simulations

In a Verification & Validation-funded project, we characterized and reproduced variability, observed in material characterization testing, by using a SIERRA Mechanics material model. Optimization was used to derive a baseline fit to the average of a collection of tension test data for 6061-T6 aluminum. Sensitivity studies and statistical software were used to determine input factors driving the response metrics.



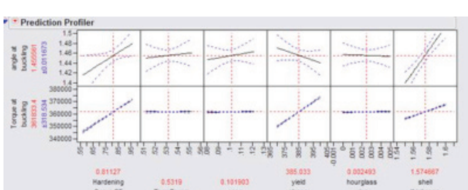
Comparison of average experimental tension test data (red curve) and +/- one standard deviation estimates (blue curve) versus average SIERRA simulation data (black circles) and +/- one standard deviation estimates (green circles) for the simulated tension test.

Ensembles of simulations using the SIERRA Mechanics code were used to fit uncertainty terms for input factors such that the variabilities in the simulated characterization tests were close to the variabilities observed in the ensemble of experimental responses. The resulting material model parameter set and the uncertainties in the parameters were then used to simulate a more complex experiment of a thin walled tube buckling in torsion. Sensitivity analysis of the tube simulations identified drivers of the buckling response.



This project leverages data collected during previous Campaign 6 funding cycles, Sandia's DAKOTA software for uncertainty quantification (UQ), sensitivity studies, and optimization, as well as training materials on the use of statistical analysis packages and approaches developed by the ASC V&V program.

SIERRA simulation of buckling behavior in a thin wall tube torsion test specimen.



Term	Prob>|t|
Intercept	<.0001*
Hardening Curve SF	<.0001*
Tear Param	0.9467
ccos	0.6612
yield stress	<.0001*
hourglass visc	0.4537
shell thickness	<.0001*

Plots from the JMP statistical analysis software package that quantify the impact of various SIERRA factors that affect the torque at which buckling occurs.

The goal of this effort is to support quantification of uncertainties in abnormal mechanical simulations where large deformations are often involved in energy dissipation. Q4FY09 work will involve application of the approach to geometries for which validation test data exists.

Los Alamos Advances Predictive Capability in Nuclear Forensics

Los Alamos National Laboratory has demonstrated leadership in simulation code capability in nuclear forensics as a result of advances in areas such as nuclear cross sections, neutron transport packages, hydrodynamics, and setup and optimization tools. For example, advances in ASC simulation tools have enabled LANL designers to perform outstandingly well in various blind-exercises over the past year or two. Generally these exercises consist of synthetic data provided to the labs, which then have 2-4 weeks to assess the design. Complete details can't be given here, except to say that LANL's assessments have been recognized for their accuracy.

The DANCE detector, a 160-element BaF2 g-array, is used to measure neutron capture and fission cross sections at the Lujan Center at Los Alamos National Laboratory. Only half of the detector is shown. b. The graph compares theoretical calculations versus data from the DANCE detector.

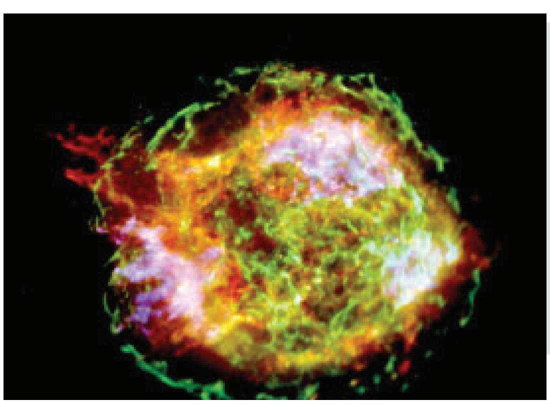
LANL established a simulation code capability for determining the design technology, materials, and possibly even the source of any nuclear weapon used against the United States or its allies. Various agencies, especially the Defense Threat Reduction Agency, NNSA, and the Department of Homeland Security, have needed a solution to this inverse problem in order to establish a full operational capability to perform nuclear forensics. LANL has worked closely with colleagues from Lawrence Livermore National Laboratory on this project.

Researchers at LANL surmounted substantial scientific challenges to complete first-ever measurements of americium cross sections, which play an important role in determining the properties of a plutonium-based device. In addition, they made significant advances in simulation codes for addressing nuclear devices whose designs likely reflect a far lower level of technology than that found in our own weapons. The figure shows detection instrumentation used at LANL.

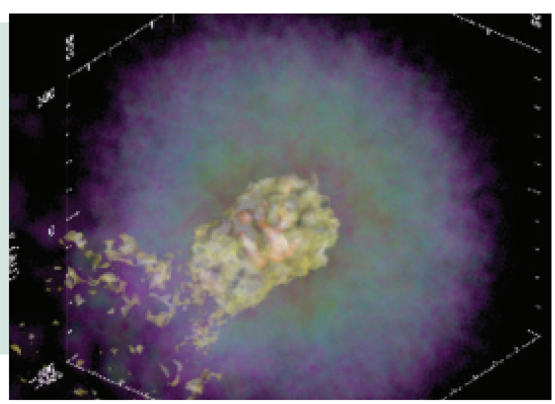
Los Alamos Pioneers Modeling Emission from Supernovae

Supernovae play an important role across a wide range of fields in physics and astronomy. They mark the endpoint in the life of stars but are an important source of energy to galaxies and play a role in the formation of new stars. They are produced in the formation of stellar-massed compact objects and, possibly, the seeds of the most massive black holes in the universe. They produce the bulk of the heavy elements in the universe and are the foundations of nuclear astrophysics.

The realization that type Ia supernovae can be used as distance estimators is one of the major scientific discoveries of the past decade. The discovery has galvanized the scientific community to use supernovae to do more than discover, but to characterize dark energy using supernovae. Many new supernova search projects have grown out of this exciting result, immensely increasing the data we have on supernovae. Both NSF (Large Synoptic Survey Telescope—LSST) and NASA/DOE (Joint Dark Energy Mission—JDEM) are sponsoring major missions to study supernovae. The figure shows a comparison of observation to computer simulation.



Experiment versus simulation: the figure on the left shows a CasA supernova remnant as observed in the sky. On the right is a 3D computer rad-hydro simulation of a supernova.



Because the amount of data from these observations is substantial and there is a dramatic increase in demand for accurate calculations of these observational properties of these explosions, researchers at Los Alamos have used the Roadrunner hybrid petaFLOP supercomputer to understand and predict light (radiation) output from supernovae as a means to help diagnose what occurs inside of supernovae. This work represents a couple of firsts in the field of nuclear particle physics: the first radiation-hydrodynamics (rad-hydro) calculation using a higher-order transport scheme, and the first multi-dimensional rad-hydro calculation of a supernova light-curve. The advanced algorithm team altered the Jayenne Project's Implicit Monte Carlo code packages to take advantage of the Cell processor on Roadrunner. The Roadrunner open-science project has added physics capability and performance functionality to the Cassio code to bear on the supernovae problem.

NNSA and DOE Supercomputers Continue to Dominate TOP500 List; Dawn Makes First Appearance

NNSA and DOE continue to dominate the TOP500 list of the world's most powerful supercomputers with 5 of the top 10 high-performance computing systems on the list released Tuesday at the International Supercomputing Conference (ISC 09) in Hamburg, Germany.

The ASC Dawn system debuted at number 9 on the latest TOP500 list.

The latest list had some surprise newcomers to the top tier of high-performance computing (HPC). An IBM BlueGene/P system, dubbed JUGENE, installed at the Forschungszentrum Julich in Germany was ranked number 3 on the list with a peak speed of just over 1 petaFLOPS. Another surprise was the appearance at number 14 of a BlueGene/P machine at King Abdullah University of Science and Technology in Saudi Arabia. Both of these machines are based on ASC's BlueGene/L technology.

The ranking of the top two systems on the list remained unchanged from last November. Roadrunner, a 1.4 petaFLOPS IBM system at Los Alamos National Laboratory, retained its top ranking, and Oak Ridge National Laboratory's Jaguar machine remains within striking distance at number 2 with its 1.3 petaFLOPS Cray system. Argonne National Laboratory's 557 teraFLOPS BlueGene/P "Solution" is ranked number 7.

BlueGene/L, with a peak speed of 590 teraFLOPS, slipped to number 5 on the list. The recently installed BlueGene/P "Dawn" system, which clocks in at a peak speed of 501 teraFLOPS, makes its first appearance on the list at number 9. Both systems serve NNSA's ASC Program. Other LLNL systems in the top 50 include Juno, Hera, and ASC Purple.

The TOP500 list, which is widely accepted as the industry standard, is released twice a year—at ISC in June and the annual Supercomputing Conference (SC) in November.

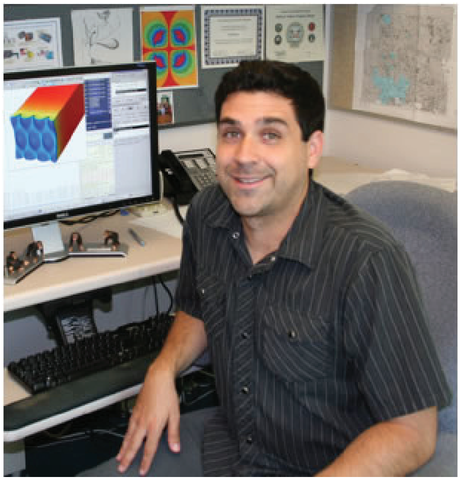
Hyperion Project Web Site Now Live

The Hyperion Project Web site is now available. [https://hyperionproject.llnl.gov/] Hyperion teams LLNL with 10 computing industry leaders to accelerate the development of powerful next-generation Linux clusters.

Matt Leininger (ICCD/Mgmt), deputy for advanced projects, notes that LLNL has received numerous requests for information about Hyperion from the academic, industry/business, and government sectors since Hyperion's formal launch. "The new Web site allows us to showcase the unique, ongoing activities on Hyperion," Matt said.

Also available on the site are graphic images in high-resolution that can be downloaded, Hyperion hardware and software configurations, links to the industry partners' Web sites, and recent news and publications.

ASC Salutes Code Physicist Rob Rieben



At the tender age of 21, Rob Rieben visited Lawrence Livermore National Laboratory as an undergraduate physics student through the Summer Institute in Applied Science program. The large-scale science performed at LLNL fascinated the budding physicist, and he decided then he would pursue his scientific career at the famous weapons lab.

After finishing his Ph.D. with an award-nominated dissertation, the results of which [https://www.llnl.gov/str/Nov07/white.html] were implemented in LLNL's massively parallel computational electromagnetics code EMSolve, Rob joined the lab as post doctoral research scientist to work on developing numerical methods for solving 3D magneto-hydrodynamics (MHD) equations. These methods were incorporated in the ASC code ALE3D. Subsequent post-doc work involved using the newly developed capabilities to perform computational modeling of complex, pulsed-power experiments.

For the past three years, Rob has managed the hydrodynamics portion of the ASC code ARES. His efforts on the ARES project have resulted in a new finite-element-based tensor artificial viscosity method, which has shown significant promise for symmetry preservation in National Ignition Facility capsule calculations. In addition, Rob is developing novel, finite-element-based methods for Lagrangian hydrodynamics to overcome long-standing issues associated with solving the Euler equations in a moving material frame.

"In a very short time, Rob has been able to make valuable contributions to the field of Lagrangian hydrodynamics and has helped energize efforts in Lagrangian methods for ASC," said Manager Brian Pudliner. "The work he's involved in right now has a great deal of potential for mitigating long-standing problems with mesh imprinting and robustness associated with traditional Lagrangian approaches."

Rob also chaired and organized the successful LLNL workshop Advanced Numerical Methods for Lagrangian Hydrodynamics, which included participation of roughly 40 experts from LLNL, Los Alamos and Sandia national laboratories, and the Atomics Weapons Establishment in England. Rob is currently serving on the international scientific organizing committee for the 2009 conference "Numerical Methods for Multi-Material Fluids and Structures."

"Since my dissertation, I've had the opportunity to work on large-scale code projects where I perform computational science on a very large scale" said Rob. "I get to think up theoretical components to solve real-world problems, on a scale completely out of the league of my previous experience. Cool."

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